

# Response of finite spin- $S$ Heisenberg chains to local perturbations

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## Abstract

We consider the properties of finite isotropic antiferromagnetic Heisenberg chains with  $S = 1/2, 1, 3/2$  spins when a weak magnetic field is applied on a few sites, using White's density matrix renormalization group (DMRG) method. For the  $S = 1$  chain there exists only one length scale in the system which determines the behavior of the one- and two-point correlation functions both around the local perturbation and near the free boundary. For the critical, half-odd-integer spin cases the exponent of the spin-spin correlation function was found to be  $\eta = 1$ , and the exponent of the decay of the site magnetization around the perturbed site is  $x_m = \eta/2$ . Close to a free boundary, however, the behavior is completely different for  $S = 1/2$  and  $S > 1/2$ .

## I. INTRODUCTION

Nowadays quantum spin chains are a very active field of research both theoretically and experimentally [1]. In early studies mostly the spectrum of magnetic excitations was considered. By now it is well known that chains described by the Heisenberg Hamiltonian with half-odd-integer spin have a gapless spectrum. In their critical behavior they belong to the same universality class, irrespective of the spin and are expected to be equivalent [2] to that of the Wess-Zumino-Witten (WZW) model with topological coupling constant  $k = 1$ . Thus, the value of the critical exponent for the algebraically decaying spin-spin correlation function is  $\eta = 1$ , independently of the value of  $S$ . On the contrary, the low energy spectrum of isotropic antiferromagnetic chains with integer spins has a gap to the lowest excited state occurring at the boundary of the Brillouin zone,  $q = \pi/a$ . This leads to the exponential decay of the spin-spin correlation function with a short correlation length.

Since the samples always contain finite chain segments, the effect of the inhomogeneity of the field distribution and the decay of the induced surface magnetization are of eminent interest for experimentalists. From a theoretical point of view a related problem, namely that of the effect of a locally applied boundary field was studied [3], but for the spin-1/2 case only.

More generally the question arises, how an external local perturbation will affect the behavior of finite or infinite spin chains. Our aim in this paper is to study the spatial dependence of the site magnetization and the spin-spin correlations in an antiferromagnetic spin- $S$  Heisenberg chain when a small magnetic field is applied locally. For this purpose we will determine, using the density matrix renormalization group (DMRG) method [4], the ground state properties of isotropic spin- $S$  finite Heisenberg chains with  $S = 1/2, 1, 3/2$  spins in a finite local field.

The layout of the paper is as follows. In Sec. II we give a short description of the results known for the  $S = 1/2, 1, 3/2$  systems. The model and a few main points of the numerical procedure applied in the course of the calculations are briefly mentioned in Sec III. The

numerical results are presented in Sec. IV. Finally Sec V. contains a brief summary.

## II. RESULTS KNOWN FOR THE SPIN-S HEISENBERG CHAINS

It is known from analytical [5] and numerical [4,6,7] studies devoted to integer spin systems that due to the finite value of the energy gap the ground-state correlation functions fall off exponentially. The most accurate value for the correlation length of the two-point correlation function  $\langle S_i^z S_{i+l}^z \rangle$  was determined by White and Huse [7]. This calculation gave  $\xi_{\text{bulk}} \simeq 6.03(1)$  for the  $S = 1$  Heisenberg chain.

They have also studied the decay length of the local magnetization near the surface. According to the valence bond model [5] of spin-1 chains in an antiferromagnet with open boundaries unpaired spins should occur at both ends of the chain. Owing to them  $\langle S_l^z \rangle$  decays exponentially as one moves towards the center of the chain, if it is calculated for the lowest  $S_T^z = 1$  state, which in the thermodynamic limit should become one of the components of the fourfold degenerate ground state. This decay length was found to be exactly the same as the correlation length in the bulk.

The analysis of critical half-odd-integer spin systems is more complicated. This is due to the existence of a marginally relevant operator in the Hamiltonian of the spin-1/2 isotropic Heisenberg antiferromagnetic chain, which leads to important logarithmic corrections to the power law decay of the spin-spin correlation function. According to the renormalization group analysis based on effective continuum models [2,8], for large  $l$  the correlation function behaves asymptotically as

$$\langle S_i^z S_{i+l}^z \rangle \sim a \times \frac{(-1)^l}{l^\eta} \left[ \log \left( \frac{l}{c} \right) \right]^\sigma - \frac{1}{4\pi^2 l^2}, \quad (1)$$

where  $a$  and  $c$  are constants,  $\eta = 1$  and  $\sigma = 1/2$ . This form was confirmed numerically by Sandvik and Scalapino [9] and recently by Hallberg *et al.* [10] using a highly accurate DMRG calculation.

If a local field is applied to a spin on the chain end, the loose edge spin is oriented and a slowly decaying magnetization develops,

$$\langle S_l^z \rangle \propto \frac{h(-1)^l}{l^{x_m}}, \quad (2)$$

where  $l$  measures the distance from the surface and  $x_m$  is the bulk scaling dimension of  $S_l^z$ . It follows from the scaling theory that  $x_m = \eta/2$ .

Recently Affleck [3] considered the critical exponent  $\eta$  of the two-point correlation function and  $x_m$  of the decay of the magnetization for the anisotropic spin-1/2 Heisenberg chain subjected to a transverse surface magnetic field. In the isotropic limit, his result for the spin-spin correlation function and the magnetization confirms Eqs. (1) and (2) with  $\eta = 1$  and  $x_m = 1/2$ .

In a finite chain, when the spins are oriented locally by an external field, this power-law decay will be modified depending on the boundary condition. The assumption of conformal invariance [11] allows us to predict the profile of the magnetization and to extract the properties of the infinite system from those of finite samples. It has been shown by Burkhardt and Xue [12] that for Ising like models on a strip of width  $L$ , conformal invariance leads to the profile

$$\langle S_l^z \rangle \sim \left[ \frac{L}{\pi} \sin \frac{\pi l}{L} \right]^{-x_m} F_{ab} \left( \cos \frac{\pi l}{L} \right), \quad (3)$$

where the function  $F_{ab}$  depends on the type of boundary applied on the two sides  $a$  and  $b$ .

In the case when the spins are fixed at  $l = 0$  and they are free at the other end,  $l = L$ , the decay of the magnetization is described by the simple form

$$\langle S_l^z \rangle \sim \left[ \frac{L}{\pi} \sin \frac{\pi l}{L} \right]^{-x_m} \left[ \cos \frac{\pi l}{2L} \right]^{x_m^s}, \quad (4)$$

where  $x_m$  and  $x_m^s$  are the bulk and surface scaling dimensions of the magnetization. Close to the free end the magnetization is proportional to

$$\langle S_l^z \rangle \sim (L - l)^{x_m^s - x_m}. \quad (5)$$

In the Ising model, where  $x_m^s = 2x_m$ , we get  $(L - l)^{x_m}$ .

One of the aims of this paper is to check whether a similar relationship holds for the Heisenberg model. We will see, that for half-odd-integer spin models with  $S > 1/2$ , although

they are critical, a new problem arises. As Ng [13] has shown, loose end spins show up not only in the valence-bond model of integer spins, where the end spin value is  $S_{\text{end}} = S/2$ , but in half-odd-integer models as well with  $S_{\text{end}} = (S - 1/2)/2$ . This was confirmed numerically by Qin *et al.* [14] using the DMRG method for spin chains with  $S = 1/2, 1, 3/2, 2$  using open boundary condition. These end spins will lead to a completely different profile of the magnetization near the free boundary for  $S = 1/2$  and  $S > 1/2$ .

Nevertheless conformal invariance can be used to check the scaling form of the spin-spin correlation function even for  $S > 1/2$  half-odd-integer spin models, as has been shown by Koma and Mizukoshi [15]. Their numerical results for  $S = 3/2$  are in agreement with the assumption that the correlations show asymptotically the same behavior as for  $S = 1/2$ . This was later confirmed by Hallberg *et al.* [16] using very extensive DMRG calculations, showing that Eq. (1) is valid for the  $S = 3/2$  chain, too, with  $\eta = 1$  and  $\sigma = 1/2$ .

### III. FORMULATION OF THE PROBLEM

In the present paper we will study the response of a 1-D spin- $S$  Heisenberg model to a small magnetic field  $h$  applied locally. The Hamiltonian of the system is written in the form

$$\mathcal{H} = \sum_i J \vec{S}_i \vec{S}_{i+1} + \mathcal{H}_{\text{local}}, \quad (6)$$

where the first term is the usual first neighbor Heisenberg model with antiferromagnetic interaction and the second term denotes the coupling of the field to a spin. In what follows we will take  $J = 1$  and measure the field relative to this coupling.

As mentioned before, effective edge spins may appear in the vicinity of the boundaries even without external field. In order to separate the magnetization induced by the field and the effect of the edge spins, the magnetic field should be applied far from the ends. In our calculations we will apply it on the central site of the chain.

In a finite field the ground state does not necessarily belong to the singlet,  $S_T = 0$ , spin sector and the spin quantum number of the ground state may change as a function of the

chain length. This may lead to complications in the finite-size scaling procedure. These difficulties can be eliminated by applying the magnetic field on two neighboring sites with opposite strength, in which case the ground state remains always in the singlet sector. We have therefore used the following expression for the local Zeeman term:

$$\mathcal{H}_{\text{local}} = hS_{N/2}^z - hS_{N/2+1}^z. \quad (7)$$

Since we are interested in the response to weak fields, we tried to remain in the regime where the local magnetization is proportional to the applied field. It turned out that for integer spins, linearity holds at least up to  $h < 0.25$ . For half-odd-integer spins this regime was found to be much smaller, thus  $h < 0.1$  fields were used for the  $S = 1/2, 3/2$  chains.

Our calculations were performed using the infinite-lattice method of DMRG. First a chain with  $N - 2$  sites is built up without field. In the case of open boundary condition we have used both the spin-reversal and the left-right reflection symmetries in order to reduce the size of the Hilbert-space of the superblock configuration. The field was introduced in the last step of the infinite-lattice method on the two sites between the left and right blocks. The number of block states kept in the calculation varied between 100 and 200. The truncation error was better than  $10^{-7} - 10^{-8}$ . As an indication of the absolute error of our calculation, we point out that in zero external field in the  $S_T^z = 0$  spin sector the largest value of the site magnetization was  $10^{-5}$ .

Since boundary effects are expected to influence the finite-size calculations we have considered both open and periodic boundary conditions. In some cases real  $S = 1/2$  spins were attached to the end of the  $S = 1$  and  $S = 3/2$  chains, further reducing the contribution of the free end spins.

#### IV. NUMERICAL RESULTS

In this section we present the results of our numerical calculations.

### A. The S=1 case

Chains up to  $N = 120$  sites were considered. This allows us to separate the boundary effects and the local magnetization induced by the field. Fig. 1 shows the absolute value of the site magnetization calculated with open boundary condition in the ground state which is a total spin singlet ( $S_T = 0$ ) state, for two values of the field applied on the central sites. The striking result of this calculation is the appearance of the end spins even in the  $S_T^z = 0$  sector for arbitrarily small finite field. It is also clearly seen in the figure that in the region around the perturbed sites, where the magnetization decays, the amplitude is proportional to the strength of the local field, while close to the free boundary the magnetization is independent of the field. As a comparison Fig. 1 also shows the site magnetization calculated for the lowest lying state in the  $S_T^z = 1$  spin sector in the absence of field.

Since the system is always gapped, an exponential decay is obtained in all cases, both near the edge and around the perturbed site. The decay length was determined, following White and Huse [7] from the quantity

$$\xi_i \equiv -1/\ln[-C(i)/C(i-1)], \quad (8)$$

where  $C(i) = \langle S_i^z \rangle$ , since it gives a clear indication of the region where the asymptotic behavior sets in. From the semi logarithmic plot used in the figure it is clear that near the edge the slopes of the curves obtained for different field values are the same. When  $M = 120$  states are kept in the DMRG we have found  $\xi_\infty \simeq 5.85(5)$ , reasonably close to the known best result for the decay length.

The analysis can be done in the same way for the decay length around the central perturbed site using

$$\xi_l \equiv -1/\ln[-C(l)/C(l-1)], \quad (9)$$

where  $l$  is measured from the perturbed site, from the middle of the chain. The same value is obtained as above. These short decay lengths ensure that the effects of the edge spins and of the locally applied field could clearly be separated.

To further clarify the origin of the nonvanishing magnetization at the boundary, real  $S = 1/2$  spins were attached to the ends of the chain with adjustable  $J_1 = J_{N-1} \equiv J_{\text{end}}$  couplings. Fig. 2 shows the site dependence of the magnetization on a semi logarithmic plot calculated for  $J_{\text{end}} = 1.5$ . It is compared to the situation when no extra spins are attached. i.e.,  $J_{\text{end}} = 0$ .

From these results it is found that the effect of the edge spin can be eliminated by the extra spin, while the magnetization is not modified far from the edge. The fit of the curves obtained with  $M = 180$  states kept leads to  $\xi_{\infty} = 5.95(3)$ , a result closer to the expected value, than that obtained for  $M = 120$ . The accuracy can be improved by fitting the quantities  $\xi_{\infty}(M)$  calculated for various values of  $M$  as a function of  $1/M$ . In the  $M \rightarrow \infty$  limit the value  $\xi_{\infty} \simeq 6.05(5)$  is found.

To complete the analysis, let us consider the effect of the field on the spin-spin correlation function. In the absence of magnetic field the two-point correlation function is usually calculated in the DMRG method by taking the two sites symmetrically with respect to the center of the chain. On the other hand, in the presence of the magnetic field acting on the site  $i = N/2$ , the correlation function  $\langle S_i^z S_{i+l}^z \rangle$  was calculated for  $i = N/2$ . Employing again Eq. (9) but with  $C(l) = \langle S_i^z S_{i+l}^z \rangle$ , and fitting the correlation functions obtained for various values of  $M$  and at different field values in the  $0 < h < 0.25$  interval, the value  $\xi_{\infty} = 5.92(5)$  is obtained for the correlation length.

Within the numerical accuracy the numbers obtained for the decay length, agree with those obtained by White and Huse [7]. We can therefore conclude that the decay length and the correlation length of the two-point correlation functions are identical and field independent. For weak fields, where linear response is valid, there is only one length scale in the system determined by the gap.

In order to have a further check, similar calculations were done also with periodic boundary condition. Our results for  $M = 20 - 180$  block states are plotted in Fig. 3. For small  $M$  values the magnetization curves are not symmetric and a minimum is observed in the curves. This is in fact due to the truncation procedure in the DMRG wave function. As



the number of the block states is increased the minimum disappears and the decay of the magnetization becomes more symmetric. Carrying out again the  $\xi(M)$  extrapolation as a function of  $1/M$ , the value of the correlation length scales to  $\xi_\infty = 6.0(1)$  in the  $M \rightarrow \infty$  limit.

It is worth mentioning that the asymmetry mentioned above is related to a similar asymmetry in the local energy  $\langle \vec{S}_i \vec{S}_{i+1} \rangle$  inside the blocks used in the DMRG method, if a relatively small number of block states is kept. This asymmetry provides therefore a better information about the real error than the truncation error [4] defined in the standard way.

### B. The $S=1/2$ case

The analysis of the critical half-odd-integer spin system is more complicated due to the logarithmic corrections. Our calculation performed on chains with some 100 sites in the interval  $0 < h < 0.1$ , where the magnetization is a linear function of the field.

First we show our results for the decay of the magnetization. The absolute value of the site magnetization calculated in the  $S_T^z = 0$  spin sector with  $M = 180$  block states and open boundary condition for  $h = 0.02$  and  $h = 0.05$  are shown in Fig. 4. Both curves were obtained for the case when the field was applied on two central sites in the configuration  $h_{N/2} = -h_{N/2+1}$ . In order to avoid complications coming from the  $1/l^2$  term of Eq. (1), only the results on even sites are shown.

Using a fit to the form in Eq. (2) by measuring the distance  $l$  from the center of the chain we have found  $A \simeq 0.37(1)$  and  $x_m = 0.49(3)$ . Since in this case the magnetization shows a downward curvature near the free end, we assumed there the form (5). We have got a good fit with  $x_m^s - x_m = 0.49(2)$ . Basically the same results were obtained when a single site was perturbed and also for other, larger values of the field. Thus we find that like in the Ising model, the relationship  $x_m^s = 2x_m$  holds for the Heisenberg model.

The effect of the field on the spin-spin correlation function has also been investigated. Following the proposal of Ref. [10] we have considered the average value

$$\overline{\omega} = \frac{1}{4}[\omega(l-1, N) + 2\omega(l, N) + \omega(l+1, N)] \quad (10)$$

to remove the  $l^{-2}$  correction of Eq. (1), where  $\omega(l, N) = (-1)^l \langle S_{i+l}^z S_i^z \rangle$ . Our data obtained for a chain with  $N = 100$  sites with  $M = 180$  block states for zero and finite ( $h = 0.25$ ) field are plotted in Fig. 5. Eq. (1) gives a good fit both without and with field, confirming that apart from logarithmic corrections the leading term in the correlation function goes as  $1/l$  even in the non-linear regime. This result also provides us with a test of the accuracy of our result when compared to those in Ref. [10].

As a further check we have considered the same problem with periodic boundary condition. The deviation of the local energy from the value obtained at the  $i = N/2$  site was of the order of  $10^{-2}$  in the interior of the block from which the system is built up in DMRG, implying that for better accuracy more block states should be used. In spite of this error we have found  $x_m = 0.48(5)$  for the decay of the magnetization and  $\eta \simeq 1$  in the spin-spin correlation function in agreement with the result obtained recently by Affleck [3].

### C. The $S=3/2$ case

It follows from our previous discussion that open boundary condition usually gives better results, in this case, however, we have to face again the problem of edge spins.

The result of the DMRG calculation performed with open boundary condition and  $h = 0.05$  for various values of the block states is plotted in Fig. 6. Two things are apparent: the contribution of the end spins causes a nonvanishing value of the site magnetization close to the chain ends and an even-odd oscillation is present even if the absolute value of the site magnetization is shown. Since the system is critical, the magnetization falls off algebraically. Therefore the effect of the field and of the end spins cannot be separated for chains for which the calculation could be done. In order to remove the contribution of the end spins we have attached real  $S = 1/2$  spins to the chain ends. The site magnetization is shown in Fig. 7. The fit to these data gives for the decay exponent  $x_m = 0.50(2)$ , the same value as obtained

for the  $S = 1/2$  case. Since according to the result of Ref. [16] the exponent of the decay of the spin-spin correlation function is  $\eta = 1$ , the relation  $x_m = \eta/2$  holds for  $S = 3/2$ , too.

The calculation of the profile for free end spins would need at least a few thousand block states as in Ref. [16].

## V. CONCLUSION

In the present paper we have considered spin- $S$  antiferromagnetic Heisenberg spin chains in a locally applied oppositely oriented magnetic field on two sites in the center of the chain, leaving the boundary spins free.

For the spin-1/2 Heisenberg chain it has been found that the linear response of the system holds only for extremely small perturbations. The exponent describing the decay of the site magnetization was found to be  $x_m = 1/2$  around the locally applied field, while  $\eta = 1$  is found for the spin-spin correlation function independently of the field thus confirming numerically, at least in the isotropic point, the analytical result obtained recently by Affleck [3]. Near the boundary the decay of the site magnetization changes character and disappears at the edge. Assuming the profile predicted by conformal invariance,  $\langle S_l^z \rangle \propto (L - l)^{x_m^s - x_m}$  with  $x_m^s = 2x_m$ , very much like in the Ising model.

For the integer spin case it was shown that linear response theory is satisfied for stronger perturbations, too. The field applied in the center of the chain, however weak it is, will orient the end spins and the site magnetization calculated in the  $S_T^z = 0$  ground state shows a dramatic increase near the ends. We have confirmed that there exists a single length scale in the system, related to the finite gap. The various bulk and surface quantities fall off exponentially with the same correlation length. In particular, we have shown that the correlation length in the two-point correlation function is identical to the decay length of the magnetization and that they are field independent.

Using periodic boundary condition we have pointed out that a better measure of the accuracy of the DMRG procedure than the truncation error could be obtained from looking

at the deviation of the local energy from its mean value.

Finally the relationship  $x_m = \eta/2$  has been shown to hold for the spin-3/2 Heisenberg chain, as well. Although this model has the same bulk critical exponents as the  $S = 1/2$  Heisenberg model, the magnetization profile is very different, resembling much more that of the  $S = 1$  model, indicating that indeed effective  $S = 1/2$  spins appear at the edges. Unfortunately, our limited computational resources did not allow us to determine the precise form of the profile.

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## REFERENCES

- [1] For a review see I. Affleck, J. Phys.: Condens. Matter, **1**, 3047 (1989).
- [2] I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989); K. Nomura, Phys. Rev. B **48**, 16814 (1993).
- [3] I. Affleck J. Phys. A: Math. Gen. **31**, 4573 (1998).
- [4] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).
- [5] I. Affleck, T. Kennedy, E. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).
- [6] S. Liang, Phys. Rev. Lett. **64**, 1597 (1990).
- [7] S. R. White and D. A. Huse, Phys. Rev. B **48**, 3844 (1993).
- [8] T. Giamarchi and H. J. Schulz, Phys. Rev. B **39**, 4620 (1989).
- [9] A. W. Sandvik and D. J. Scalapino, Phys. Rev. B **47**, 12333 (1993).
- [10] K. Hallberg, P. Horsch, and G. Martínez, Phys. Rev. B **52**, R719 (1995).
- [11] For a review see J. L. Cardy in *Phase Transition and Critical Phenomena*, Vol. 11., C. Domb and J. L. Lebowitz, eds. Academic Press, London, (1987).
- [12] T. W. Burkhardt and T. Xue Phys. Rev. Lett. **66**, 895 (1991).
- [13] T.-K. Ng, Phys. Rev. B **50**, 555 (1994).
- [14] S. Qin, T.-K. Ng, and Z.-B. Su, Phys. Rev. B **52**, 12844 (1995).
- [15] T. Koma and N. Mizukoshi, J. Stat. Phys. **83**, 661 (1996).
- [16] K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996).

## FIGURES

FIG. 1. The absolute value of the site magnetization calculated in the  $S_T^z = 0$  spin sector of the ground state for an  $S = 1$  spin chain with  $N = 120$  sites for two values of the locally applied field. For comparison the magnetization obtained in the lowest lying state of the  $S_T^z = 1$  spin sector without field is also shown.

FIG. 2. The same as Fig. 1. for one value of the field for the case when an extra  $S = 1/2$  spin is coupled to the chain ends with the exchange coupling  $J_{\text{end}}$ . Only the values for the left half of the chain are plotted.

FIG. 3. The same as Fig. 1. for one value of the field but for periodic boundary condition, for various values of the number of states kept. The straight lines are fits with exponential decay.

FIG. 4. The site magnetization of a  $S = 1/2$  spin chain obtained in the  $S_T^z = 0$  spin sector with open boundary condition.  $N = 120$ ,  $M=180$   $h = 0.02$  and  $h = 0.05$ . The solid lines correspond to our fits explained in the text.

FIG. 5. The averaged spin-spin correlation function of the  $S = 1/2$  spin chain obtained in the  $S_T^z = 0$  spin sector with open boundary condition in the absence of the field and for  $h = 0.25$ . The solid lines correspond to our fits explained in the text.

FIG. 6. The site magnetization of  $S = 3/2$  magnetic chain with  $N = 60$  sites calculated for various values of  $M$  with open boundary condition.

FIG. 7. Same as Fig. 6. but with real  $S = 1/2$  spins attached to the chain ends.